SOME EXACT EXCITED STATES IN A LINEAR ANTIFERROMAGNETIC SPIN SYSTEM

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Exact expressions are derived for some excited states in a linear quantum spin system for which the exact ground state has been studied in the last decade.

1. Hamiltonian and notation. We consider a linear antiferromagnetic lattice which contains a next nearest neighbour interaction (NNN) with half the strength of the nearest neighbour interaction (NN). The hamiltonian is of the Heisenberg type:

$$H = 4\sum_{i=1}^{2N} \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + 2\sum_{i=1}^{2N} \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2} , \qquad (1)$$

$2N$ is the number of spins ($S_i = 1/2$).

Assuming periodic boundary conditions, we put $\boldsymbol{S}_{2N+i} = \boldsymbol{S}_i$ for every lattice site i. For convenience, the chain is divided into N cells of 2 spins, and H can be split up into two parts [1–4]:

$$H_0 = \sum_{k=1}^{N} H_{0k} \quad \text{and} \quad H' = \sum_{k=1}^{N} H'_{k,k+1} , \qquad (2)$$

where

$$H_{0k} = 4\boldsymbol{S}_{2k-1} \cdot \boldsymbol{S}_{2k} = 2[(\boldsymbol{S}_{2k-1} + \boldsymbol{S}_{2k})^2 - \tfrac{3}{2}] \qquad (3)$$

describes the internal interaction in the kth cell, containing the spin pair $(\boldsymbol{S}_{2k-1}, \boldsymbol{S}_{2k})$, and

$$\begin{aligned} H'_{k,k+1} &= 4\boldsymbol{S}_{2k} \cdot \boldsymbol{S}_{2k+1} \\ &\quad + 2(\boldsymbol{S}_{2k-1} \cdot \boldsymbol{S}_{2k+1} + \boldsymbol{S}_{2k} \cdot \boldsymbol{S}_{2k+2}) \qquad (4) \\ &= 2(\boldsymbol{S}_{2k-1} + \boldsymbol{S}_{2k}) \cdot \boldsymbol{S}_{2k+1} + 2\boldsymbol{S}_{2k} \cdot (\boldsymbol{S}_{2k+1} + \boldsymbol{S}_{2k+2}) \end{aligned}$$

describes the coupling between the kth and the $(k+1)$-st cell, which contains 1 nn interaction and 2 nnn interactions.

2. Eigenstates and eigenvalues of H_{0k}. The eigenstates of H_{0k} are chosen to be simultaneous eigenstates of $(\boldsymbol{S}_{2k-1} + \boldsymbol{S}_{2k})^2$ and $S^z_{2k-1} + S^z_{2k}$, and can thus be labeled by the total spin S_k and its z-component M_k. In the two-spin representation of the kth cell, the spectrum of H_{0k} splits up into a singlet and a triplet, as is shown in table 1.

3. The ground state of H. Consider the product

$$|\Phi_0\rangle = |0\rangle_1 \otimes |0\rangle_2 \otimes ... \otimes |0\rangle_N = \prod_{k=1}^{N} |0\rangle_k . \qquad (5)$$

$|\Phi_0\rangle$ turns out to be not only the ground state of H_0, but also an eigenstate of $H = H_0 + H'$ with the lowest possible eigenvalue $E_0 = -3N$. There are two eigenstates of H, corresponding with this lowest possible eigenvalue. The other one is found by translation over one lattice spacing [1–4].

4. Shorthand notations. Let $|\Phi_k(M)\rangle$ be a many-cell state in which only the kth cell is in a triplet state (with quantum number M). In the same way $|\Phi_{kl}(M,M')\rangle$ denotes a state with only two cells (k,l) in a triplet state (M resp. M'). In other words, if a particular cell j does not appear in the notation of a many-cell state, it is assumed to be in the cell ground state, i.e. in the

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Table 1

	S_k	M_k	
$\|0\rangle_k = 2^{-1/2}(\|+-\rangle_k - \|-+\rangle_k)$ a)	0	0	$H_{0k}\|0\rangle_k = -3\|0\rangle_k$
$\|1M\rangle_k = \|++\rangle_k$	1	1	$H_{0k}\|1M\rangle_k = \|1M\rangle_k$
$= 2^{-1/2}(\|+-\rangle_k + \|-+\rangle_k)$	1	0	
$= \|--\rangle_k$	1	−1	

a) $|+-\rangle_k$ denotes a cell state with spin up and down on sites $2k-1$, $2k$ respectively, and so on.

singlet state $|0\rangle_j$. Finally,

$$|SM\rangle_{kl} = \sum_{M_1,M_2} \langle 1M_1\,1M_2|11SM\rangle|\Phi_{kl}(M_1,M_2)\rangle\,,$$

$$S=0,1,2\,,\quad M=-S,-S+1,\ldots,S-1,S\,, \tag{6}$$

describes the addition of the cell spins of the cells k and l, when both cells are in a triplet state. $\langle 1M_1\,1M_2|$ $\times\,|11SM\rangle$ is a Clebsch–Gordan coefficient [5].

5. *Some excited states.* Excited states can be constructed exactly, by taking appropriate linear combinations of some basic states $|\Phi_k(M)\rangle$ and $|SM\rangle_{kl}$. In order to prove that those are exact eigenstates of H, one has to figure out how H' acts on the basic states. Using conventional Clebsch–Gordan technology, and applying the Wigner–Eckart theorem [5] for irreducible tensor operators, one finds:

$$H'_{k,k+1}|\Phi_0\rangle = 0\,,$$

$$H'_{k,k+1}|\Phi_k(M_1)\rangle = \sqrt{2}|1M_1\rangle_{k,k+1}\,,$$

$$H'_{k,k+1}|\Phi_{k+1}(M_2)\rangle = \sqrt{2}|1M_2\rangle_{k,k+1}\,,$$

$$\begin{aligned} &H'_{k,k+1}|\Phi_{k,k+1}(M_1,M_2)\rangle \\ &\quad = -4\sqrt{3}\sum_{\mu M_1' M_2'}\langle 1\mu\;1{-\mu}|1100\rangle\langle 1\mu\,1M_1|111M_1'\rangle \\ &\quad\times\langle 1{-\mu}\,1M_2|111M_2'\rangle|\Phi_{k,k+1}(M_1',M_2')\rangle \\ &\quad+\sqrt{2}\sum_{M'}\langle 1M_1\,1M_2|111M'\rangle(|\Phi_k(M')\rangle+|\Phi_{k+1}(M')\rangle), \end{aligned} \tag{7}$$

$$H'_{k,k+1}|SM\rangle_{k,k+1} = [S(S+1)-4]|SM\rangle_{k,k+1}$$
$$+\sqrt{2}\delta_{S1}[|\Phi_k(M)\rangle + |\Phi_{k+1}(M)\rangle]\,.$$

δ_{ij} is the Kronecker delta symbol.

With the help of these equations, the following set of eigenstates has been constructed for the full hamiltonian:

(1) A triplet ($S=1$) of eigenstates with energy $E=-3N+4$, containing only states with one excited cell:

$$|\psi_{1M}\rangle = \frac{1}{\sqrt{N}}\sum_{k=1}^{N}(-1)^k|\Phi_k(M)\rangle\,,\quad N\text{ even}\,. \tag{8}$$

(2) A singlet ($S=0$), with energy $E=-3N+4$, containing only states with two excited cells:

$$|\phi\rangle = \frac{1}{\sqrt{N}}\sum_{k=1}^{N}(-1)^k|00\rangle_{k,k+1}\,,\quad N\text{ even}\,. \tag{9}$$

(3) A triplet ($S=1$), with energy $E=-3N+8$, containing only states with one or two excited cells:

$$|\chi_{1M}\rangle = \frac{1}{N}\Big[-\sum_{k=1}^{N}|\Phi_k(M)\rangle + \sqrt{2}\sum_{1\leqslant k<l\leqslant N}(-1)^{k+l}|1M\rangle_{kl}\Big]\,,\quad N\text{ odd}\,. \tag{10}$$

All states are normalized to 1.

6. *Concluding remarks.* The presented excited states correspond to exact eigenstates of the hamiltonian H given in (1), and are characterized by a fixed maximum number of cell excitations. Recently, Shastry and Sutherland [3] investigated, for the same system, excited states of a different nature. They considered the two phases of the system represented by singlet pairs $(2k-1,2k)$ and $(2l,2l+1)$ respectively, separated by defects, i.e. single spins. To meet periodic boundary conditions the number of defects should be even. In particular they analyzed states with two defects and

solved for these states an approximate secular problem, resulting in elementary excitations with the same wave number, energy and spin as those represented by the states $|\psi_{1M}\rangle$ and $|\phi\rangle$ of our formulas (8) and (9) respectively. This agreement merits further detailed analysis.

For further exact results in linear quantum spin systems we may refer to refs. [6,7].

7. Two-dimensional systems. Using the same method, it is also possible to construct exact eigenstates for some two-dimensional versions of the presented hamiltonian. Details will be published in a separate paper.

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